

Local moment versus Kondo behavior of the 4*f*-electrons in rare-earth iron oxypnictides

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We consider the role played by the 4*f* states in the rare-earth oxyarsenides REOFeAs (RE=Ce,Pr,Nd) and the oxyphosphate CeOFeP, using a first-principles technique that combines the local density approximation and dynamical mean-field theory (LDA+DMFT). In the Pr and Nd compounds, the 4*f* states are located well below and above the Fermi level E_F , and essentially do not interact with the iron 3*d* bands located near E_F , resulting in local moment behavior. In the Ce compounds, our results reveal a qualitatively different picture, with the 3*d*-4*f* hybridization being sufficiently strong to give rise to an observable Kondo screening of the local 4*f* moment. Our LDA+DMFT electronic structure calculations allow us to estimate the Kondo temperature T_K for both CeOFeP and CeOFeAs. For the phosphate, the order of magnitude of our estimate is consistent with the experimental observation of $T_K \simeq 10$ K. At ambient pressure, T_K is found to be negligibly small for CeOFeAs. Under applied hydrostatic pressure, we predict an exponential increase of T_K which reaches values comparable to the superconducting $T_c \simeq 40$ K at pressures above 10 GPa. We conjecture that the competition between the Kondo effect and superconductivity may be at the origin of the monotonous decrease of T_c observed in CeOFeAs under pressure. We argue that the quantitative aspects of this competition are inconsistent with a weak-coupling BCS description of the superconductivity in the oxyarsenides.

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The discovery of the REO_{1-x}F_xFeAs superconductors with a transition temperature up to $T_c = 55$ K [1, 2, 3, 4, 5, 6] and the observation of superconductivity also in oxygen deficient REFeAsO_{1-δ} [7] has triggered enormous efforts, both experimentally and theoretically, aimed at understanding the electronic properties of rare earth iron oxypnictides. The evolution of T_c along the series of rare earth elements, and possible correlations with structural properties have attracted particular interest. While LaO_{1-x}F_xFeAs has a T_c of 26 K, the critical temperature is drastically increased by replacing La by other rare earth ions (RE=Ce,Pr,Sm,Nd,Gd), up to ~ 55 K for Sm. Possible correlations between the evolution of T_c with changes in the structural parameters due to decreasing size of the rare-earth ions along the series have been reported in the literature [7, 8].

On the theoretical side, most *ab initio* studies have so far concentrated on the La compound. To our knowledge, only the work of Nekrasov *et al.* [9] has addressed the question of how the electronic structure of REOFeAs changes upon rare-earth substitution. On the basis of LDA calculations, these authors obtained essentially identical electronic structures for all the REOFeAs compounds considered (with RE=La,Ce,Pr,Nd,Sm,Y). In their work [9], the 4*f* shells of the rare-earths were treated as core states. However, an intriguing question is whether the low-energy electronic structure of REOFeAs might be modified along the rare earth series, due to the hybridization between the Fe 3*d* band and the localized 4*f* states of the rare earth ions. This possibility has not

been so far investigated in the literature. Meanwhile, a Kondo screening of the Ce local magnetic moment on the 4*f* shell has been observed in the CeFePO compound, an homologue of CeFeAsO, with a reported Kondo temperature $T_K = 10$ K [10]. This implies the existence of an hybridization between the Fe 3*d* bands in the vicinity of E_F and the localized Ce 4*f* states. The discovery of the Kondo effect in CeFePO raises the possibility that the Re4*f*-Fe3*d* hybridization might similarly lead to a Kondo screening of the RE local moment in some of the oxyarsenide compounds.

In order to investigate the 4*f* states and their interaction with other bands, a many-body treatment of the strong Coulomb interaction between 4*f* electrons is necessary. Therefore we have employed the combined local density approximation and dynamical mean-field theory (LDA+DMFT) approach [11, 12] to study properties of 4*f* states in CeOFeP and REOFeAs (RE=Ce,Pr,Nd). We show that in the Pr and Nd compounds the 4*f* states are very localized, leading to unscreened local moments. The occupied 4*f* states are located well below the 3*d*-Fe states, and the unoccupied ones well above.

We find that the situation is different, however, for the Ce compounds CeOFePn (Pn=P and As), for which the occupied 4*f* band is located at the bottom or just below the bottom of the 3*d*-Fe states. The resulting hybridization leads to Kondo screening of the 4*f* Ce local moment at low T. We estimate the Kondo temperatures of CeOFeP, and find that the order of magnitude is consistent with experiments. We predict a rapid increase of

the (very low) Kondo scale of CeOFeAs as a function of pressure, due to the contraction of the Fe-Ce interatomic distance and to the corresponding increase of the f - d hybridization. Moreover, we conjecture that the Kondo effect in CeOFeAs may be at the origin of the rather rapid suppression of T_c under pressure observed in doped CeOFeAs [13] (which is in sharp contrast to the behaviour under pressure of LaOFeAs [13] at a similar doping level).

We have employed the LDA+DMFT approach using the recently developed fully-selfconsistent framework described in [14]. The local self-energy of the $4f$ shell is computed according to the DMFT prescription and by employing the atomic (Hubbard-I) approximation [15]. This approach to local correlations has been shown to be appropriate for the localized $4f$ shells of rare-earth compounds [14]. We have used the full four-index U matrix for the local Coulomb interaction. The spin-orbit coupling and splitting of the bare $4f$ levels due to the crystal field were taken into account. Our calculations are performed for the paramagnetic state and at zero temperature.

In order to determine the value of the local Coulomb interaction U on the $4f$ shell, we have performed constrained LDA calculations. We obtain a value of about 9.7 eV for both CeOFeAs and CeOFeP. This is substantially larger than the usual range of U values for pure Ce. This result can be explained by the quasi two-dimensional environment of the rare-earth sites in the case of oxypnictides, with only four nearest-neighbours present, which leads to a rather poor screening of the local Coulomb interaction. Values of the Slater integrals F^2 , F^4 , and F^6 , which are known to be weakly dependent on crystalline environment, have been taken from the optical measurements of [16]. The corresponding values of the exchange parameter J are equal to be 0.69, 0.73, and 0.77 eV for Ce, Pr, and Nd, respectively. For the double counting correction, we have employed the fully-localized limit expression $U(N_f - 1/2) - J(N_f/2 - 1/2)$, where the occupancy N_f in the atomic limit and at zero temperature is equal to 1, 2, and 3 for Ce, Pr, and Nd, respectively.

All calculations have been carried out at the experimental lattice parameters a and c [2, 3, 4]. An unusual sensitivity of the low-energy electronic structure of iron oxypnictides to the vertical distance between the Fe and As planes z_{As} has been pointed out in the literature [17, 18]. However, in the present work, we mainly focus on high-energy features of the electronic structure, particularly on the $4f$ bands and their interaction with other bands. Those features are not expected to be very sensitive to small changes in the Fe-As distance, they may rather show some sensitivity with respect to the vertical position of the rare-earth plane z_{RE} , which is almost constant along the series [8, 19, 20]. Thus the experimental values of the internal parameters z_{As} and z_{RE} for LaOFeAs [21] have been used for all oxyarsenides stud-

ied, while CeOFeP has been computed with the internal parameters fixed at their experimental values for PrOFeP [22].

Because the atomic Hubbard-I approximation to strong correlations is not able to capture directly the Kondo effect, we have employed the approach of Gunnarsson and Schönhammer [23] to calculate the Kondo temperature. Within this approach the Kondo temperature is given (in the Kondo regime) by the following expression:

$$T_K = D e^{-\frac{|\epsilon_f|}{N_f \rho_0 V_{cf}^2}}, \quad (1)$$

where ϵ_f is the average position of the occupied $4f$ level, ρ_0 is the density of states at the Fermi level, N_f is the f band degeneracy, V_{cf} is the average hybridization matrix element between the $4f$ level and the conduction band, D is the bandwidth of the occupied part of the conduction band. As shown in [23], the spin-orbit splitting yields a rather small correction to T_K and can be neglected, so that we take $N_f=14$. The value of V_{cf}^2 can be estimated from the imaginary part of the DMFT hybridization function at E_F , which reads:

$$\text{Im}\Delta(E_F) = \text{Im} \sum_{\mathbf{k}} \frac{|V_{cf}^{\mathbf{k}}|^2}{E_F - \epsilon_{\mathbf{k}}} \approx \pi \rho_0 V_{cf}^2, \quad (2)$$

where $\epsilon_{\mathbf{k}}$ are the conduction band states. For a degenerate case, the average value of V_{cf}^2 can be extracted from $\text{Tr} \text{Im}\Delta(E_F)/N_f$. An accurate evaluation of the parameters entering in the exponential factor in (1) is necessary to obtain any reasonable estimate of T_K . Thus we have employed a 9000 \mathbf{k} -point mesh in the Brillouin zone in our LDA+DMFT calculations in order to evaluate the average hybridization V_{cf} and the $4f$ level position ϵ_f . To obtain an accurate value of the density of states at the Fermi level, we use a Full-Potential APW+local orbitals code[24] with the $4f$ states in the core. We have checked that all the values used in calculation of T_K are converged with respect to the \mathbf{k} -point mesh.

First, we discuss the LDA+DMFT electronic structure of the CeOFeP compound in connection with the Kondo screening of the Ce local magnetic moments observed experimentally in this compound. In the upper panel of Fig. 1 the LDA+DMFT spectral function at $U - J = 9$ eV (in red) is superimposed to the band structure obtained by treating the Ce $4f$ states as core (in blue). The empty Ce $4f$ states (the upper Hubbard band) form rather dispersionless bands between 6 and 9 eV above E_F hybridized to a certain degree with the Ce $5d$ band. The occupied part (the lower Hubbard band) of the Ce $4f$ states is located at about 1.8-2 eV below E_F . It hybridizes substantially with the p states of mostly oxygen character at the top of the As/O p band, causing a downward shift of 0.5 eV of the oxygen $2p$ band that was located at ~ 2.3 eV in the LDA with f in core band structure. In the lower panel the corresponding partial density

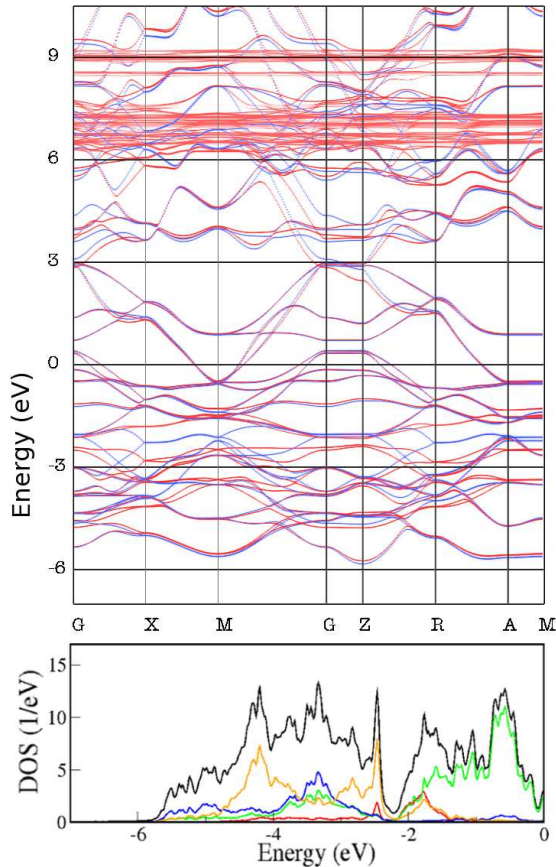


Figure 1: Electronic structure of CeOFeP obtained within LDA with the $4f$ states treated as core (blue line) and within LDA+DMFT (red line). The $4f$ states of RE form a rather dispersionless upper Hubbard band 6-9 eV above the Fermi energy. The lower Hubbard band is more dispersed due to hybridization with O $2p$ and Fe $3d$. It is located between -1.8 and -2 eV. In the lower panel the density of occupied states is displayed, with the total, partial Ce $4f$, Fe $3d$, pnictogen p and O $2p$ shown by black, red, green, blue, and orange curves, respectively. One may notice a rather strong hybridization between the O $2p$ states at the top of p band and the occupied $4f$ states.

of (occupied) states is depicted. Note that, because the Hubbard-I approximation does not capture the Kondo peak, the LDA+DMFT (Hubbard-I) spectral function in Fig. 1 should be viewed as the band structure for $T > T_K$.

From the imaginary part of the Ce $4f$ hybridization function we have obtained $V_{cf}=116$ meV, while $\epsilon_f=-2.0$ eV, $\rho_0=1.85$ (eV \times formula unit) $^{-1}$, and $D\sim 2$ eV for the Fe $3d$ bands, resulting in an estimate of $T_K \simeq 77$ K. This is a reasonable order of magnitude in comparison to the experimental result $T_K=10$ K of Brüning *et al.* [10], given that our estimate for T_K is obtained for the single impurity case. Indeed, the corresponding T_K for the Kondo lattice is expected to be reduced by at least a factor of 2 for the approximately half-filled conduction (Fe $3d$)

band under consideration[25]. Our estimates for ϵ_f and $\rho_0 V_{cf}^2=25$ meV also compare well with the corresponding values of -2.4 eV and 19 meV, respectively, obtained for CeCu₂Si₂ by Kang *et al.* [26] from a fit to the experimental PES spectra. As noted in Ref. [10], CeCu₂Si₂ and CeOFeP have about the same Kondo temperature and Sommerfeld coefficient γ of the specific heat.

We have also performed LDA+DMFT calculations for CeOFeP using the "standard" value of 6 eV for the U parameter of pure Ce $4f$. Those calculations predict the lower Hubbard band to be much closer to the Fermi level, with $\epsilon_f \simeq -0.5$ eV. This would lead to a unrealistically high Kondo temperature for CeOFeP, even if one takes into account necessary corrections to (1) due to deviation from the Kondo regime (mixed valence behavior) for small values of $|\epsilon_f|$. Therefore, the constrained LDA value of the local Coulomb interaction $U - J=9$ eV provides a better description of the Kondo behaviour in CeOFeP as compared to the usual choice of U for pure Ce. We used the same value to study the oxyarsenides.

In Fig. 2, we compare the LDA+DMFT band structures of stoichiometric CeOFeAs, PrOFeAs and NdOFeAs with the band structures obtained for the same compounds within LDA by treating the rare-earth $4f$ states as core. Differences between the LDA+DMFT and LDA-with- $4f$ -in-core electronic structures are especially pronounced well above E_F , where the unoccupied $4f$ states form a set of dispersionless bands in the range of energies from 6 to 9 eV, from 4 to 8 eV, and from 3 to 7 eV for the Ce, Pr, and Nd compounds, respectively. The width of about 3 eV of those upper Hubbard bands is due to multiplet splittings associated with the exchange and spin-orbit interactions. The occupied $4f$ states are located in the range of energies from -2.3 to -3 eV in CeOFeAs, from -4 to -5 eV in PrOFeAs, and below -6 eV for NdOFeAs. Similarly to the case of CeOFeP, the occupied $4f$ states hybridize rather strongly with the oxygen p states, which are located mainly at the top of the As $4p$ /O $2p$ band. This $4f$ - $2p$ hybridization leads to some modifications at the top of the O/As p band in comparison with the f -in-core band structure. In contrast, the Fe $3d$ bands are hardly modified by the interaction with the $4f$ states, as one may see in the upper panel of Fig. 2 where blue and red bands corresponding to Fe (close to the Fermi level) essentially coincide. From these results, we conclude that the $4f$ electrons behave as unscreened localized moments in the Pr- and Nd- compounds.

In contrast, for CeOFeAs, the lower Hubbard band is located rather close to the Fe $3d$ bands (see the corresponding DOS on Fig. 2). Thus, in analogy to the case of CeOFeP, in CeOFeAs one might expect to observe a Kondo screening of the $4f$ local moment. We have estimated the Kondo temperature in CeOFeAs using formula (1), and the resulting values are given in the first row of Table I. With $D \simeq 2$ eV for the Fe $3d$ bands, this leads to a value of T_K of order 10^{-4} K. Thus, T_K in CeOFeAs is

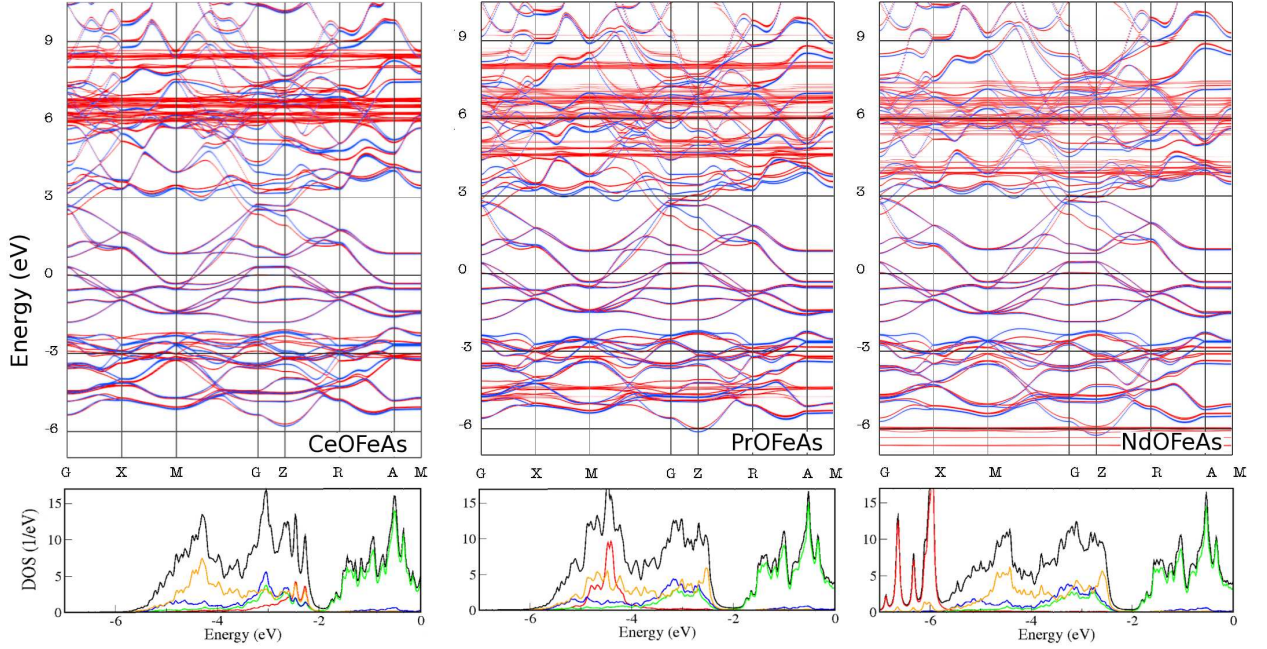


Figure 2: Electronic structure of stoichiometric iron oxyarsenides obtained within LDA with the $4f$ states treated as core (blue line) and within LDA+DMFT (red line). The empty $4f$ states of RE form a rather dispersionless upper Hubbard band significantly above the Fermi energy. The lower Hubbard band is located just below the bottom of the Fe $3d$ band, in the middle of the O/As p band and below the p band in CeOFeAs, PrOFeAs, and NdOFeAs, respectively. The lower panel displays the corresponding densities of states, the color coding is the same as in Fig. 1

negligible in comparison to the magnetic ordering temperature for the Ce local moments, which was measured to be about 5 K in this compound[3]. This drastic reduction of the Kondo scale (by about 5 orders of magnitude!) in comparison to T_K for CeOFeP is mainly due to a substantially weaker $3d$ - $4f$ hybridization in CeOFeAs. This decrease of the d - f hybridization is rather expected, as the Fe-Ce distance is larger in CeOFeAs than in CeOFeP.

In order to investigate the behavior of the Kondo scale under applied pressure we have estimated the corresponding change in volume of CeOFeAs. Methods based on the atomic sphere approximation can not reliably describe elastic properties of a complex crystal structure. One may notice that the structural parameters of CeOFeAs and LaOFeAs are rather similar, while the $4f$ states of Ce, being still essentially localized, are not expected to affect substantially the elastic properties of CeOFeAs. Therefore, for CeOFeAs we have adopted the theoretical elastic constants computed for LaOFeAs [27] within a full-potential approach. With those elastic constants the relative values of the lattice parameters $a/a_0(c/c_0)$ of CeOFeAs (where a_0 and c_0 are the corresponding values at zero pressure) are equal to 0.985(0.978), 0.970(0.956), and 0.955(0.934) under hydrostatic pressure of 5, 10, and 15 GPa, respectively. Anisotropy of the elastic constants leads to a substantially larger relative contraction for the c -parameter com-

Table I: The average hybridization V_{cf} and $4f$ level position ϵ_f , density of states at the Fermi level ρ_0 , and Kondo temperature T_K in CeOFeAs as function of applied pressure

P(GPa)	V_{cf} (meV)	ϵ_f (eV)	ρ_0 (eV*formula unit) ⁻¹	T_K (K)
0	77	-3.03	2.0	0.0003
5	90	-2.74	1.86	0.067
10	111	-2.38	1.77	9.8
15	129	-2.04	1.70	137.0

pared with the one for a .

In Table I we list, as a function of applied pressure, the values of the average hybridization V_{cf} and $4f$ -level position ϵ_f obtained within LDA+DMFT as well as the density of states at the Fermi level. One may see that V_{cf} grows substantially with increasing pressure, while the $4f$ -level position is shifted towards the Fermi level. The reduction of the Ce-Fe distance naturally leads to an increase in the corresponding hybridization matrix elements, the contraction in the Ce-O distance further enhances the strong O $2p$ -Ce $4f$ hybridization, leading to the upwards shift of ϵ_f . The Fe $3d$ bandwidth increases as well under pressure, leading to a drop in ρ_0 . However the effects due to the sharp rise in V_{cf} are obviously the most important, leading to a reduction of $|\epsilon_f|/(\rho_0 V_{cf}^2)$ in formula (1) and to a corresponding (almost exponential) increase of the Kondo temperature as a function of pres-

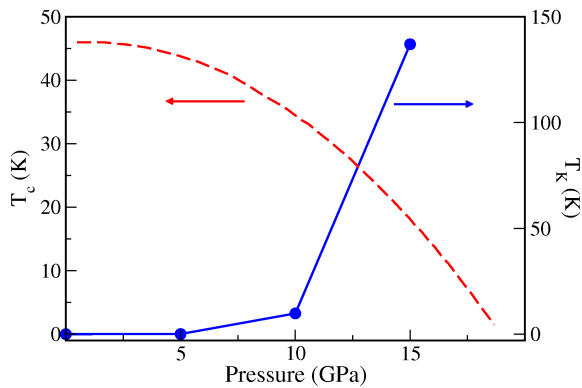


Figure 3: Experimental evolution of the superconducting transition temperature T_c in $\text{CeO}_{0.88}\text{F}_{0.12}\text{FeAs}$ under applied pressure [13] (red dashed curve) and our theoretical estimate for the corresponding evolution of the Kondo temperature T_K in CeOFeAs (blue solid curve).

sure (see Table I). Hence, T_K raises from the negligible value of 10^{-4} K at ambient pressure to a value of order 100 K under an applied pressure of 15 GPa.

Within our approach one may only obtain a rather crude estimate for T_K . But our *qualitative conclusions* should be rather robust: as the pressure increases the Kondo temperature exhibits an exponential growth, from values which are negligible compared to the superconducting transition temperature T_c at ambient pressure, up to values of the same order of magnitude as T_c at pressures above 10 GPa. It is interesting to contrast the predicted enhancement of T_K under pressure with the behavior of T_c observed experimentally for $\text{CeO}_{0.88}\text{F}_{0.12}\text{FeAs}$ [13] (see Fig. 3). In contrast to $\text{LaO}_x\text{F}_{1-x}\text{FeAs}$ at a very similar doping level, for which T_c raises with increasing pressure up to 5 GPa before starting to decrease rather slowly [13], in $\text{CeO}_{0.88}\text{F}_{0.12}\text{FeAs}$ one observes a monotonous and rather steep decrease of T_c with increasing pressure. The superconducting transition is actually completely suppressed at pressures of about 20 GPa. As one may see in Fig. 3, a rapid reduction of T_c sets in at pressures (above 5 GPa), at which T_K starts to reach values of order of a few degrees Kelvin. Thus, we may conjecture that the rapid suppression of superconductivity observed in the doped CeOFeAs under pressure is due to the corresponding stabilization of a competing heavy-fermion phase with Kondo-screened local moments of the Ce shell.

The competition between the Kondo effect and s -wave superconductivity has been investigated theoretically in Ref. [30], in the framework of the periodic Anderson model. This study concluded that with $T_K > T_{c0}^2/W$ (where T_{c0} is the transition temperature in the absence of the Kondo effect and W is the bandwidth of the conduction band), the s -wave superconductivity becomes rapidly suppressed, with T_c decreasing exponentially as a

function of T_K . This expresses the competition between the Kondo screening energy ($\sim T_K$) and the condensation energy $\sim T_{c0}^2/W$ of a weak-coupling BCS superconductor. In our case the threshold value of $T_K = T_{c0}^2/W$ is of order of 0.1 K. However, our estimates of T_K lead us to conclude that while the Kondo effect may be responsible for a rather rapid suppression of the superconductivity in $\text{CeO}_x\text{F}_{1-x}\text{FeAs}$ under applied pressure, the actual superconducting phase is still much more robust than what would be predicted by the theory in Ref. [30]. This points out to important differences between the nature of the superconductivity of the rare-earth iron oxyarsenides and that of a weak-coupling BCS superconductor.

In conclusion, our study reveals that while for the heavier rare-earths the electrons in the $4f$ shell of rare-earth oxyarsenides behave as unscreened local moments, the Cerium-based compounds behave in a different manner. There, a competition between Kondo screening and superconductivity takes place under applied pressure. This may be responsible for the suppression of superconductivity under applied pressure in the cerium-based compounds, and suggests that the competing phase at large pressure should be a heavy-fermion state with a moderate effective-mass enhancement. Orders of magnitude suggest however that the Kondo effect is less detrimental to superconductivity in these compounds than for a weak-coupling BCS superconductor, hence providing indirect evidence for the unconventional nature of superconductivity in the oxyarsenides. This competition between superconductivity and a heavy-fermion state deserves further theoretical and experimental investigations.

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